Fumaric acid, 3,3-dimethylbut-2-yl heptadecyl ester

Inchi: InChI=1S/C27H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-30-25(28)21-22-

InchiKey: OHGSCHFZBKKXIW-QURGRASLSA-N

Formula: C27H50O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-210.76	kJ/mol	Joback Method
hf	-987.02	kJ/mol	Joback Method
hfus	60.52	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.935		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	970.23	K	Joback Method
tc	1191.32	K	Joback Method
tf	520.71	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.79	J/mol×K	970.23	Joback Method
cpg	1402.63	J/mol×K	1007.08	Joback Method
cpg	1422.02	J/mol×K	1043.93	Joback Method
cpg	1440.05	J/mol×K	1080.78	Joback Method
cpg	1456.81	J/mol×K	1117.62	Joback Method
cpg	1472.39	J/mol×K	1154.47	Joback Method
cpg	1486.87	J/mol×K	1191.32	Joback Method
dvisc	0.0003432	Pa×s	520.71	Joback Method

dvisc	0.0001356	Pa×s	595.63	Joback Method
dvisc	0.0000659	Pa×s	670.55	Joback Method
dvisc	0.0000371	Pa×s	745.47	Joback Method
dvisc	0.0000231	Pa×s	820.39	Joback Method
dvisc	0.0000156	Pa×s	895.31	Joback Method
dvisc	0.0000112	Pa×s	970.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348716&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume